Aluminium triflate as a Lewis acid catalyst for the ring opening of epoxides in alcohols

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Supplementary Information

All compounds were determined to be >99% pure on the basis of GC-FID analyses (total peak area), taken together with 'clean' NMR spectra, after isolation by column chromatography and/or vacuum distillation. Copies of three ^{13}C NMR spectra are included as examples. Regioisomers were distinguished on the basis of gHMBC and gHMQC NMR experiments.

2-Methoxy-2-phenylethanol, IR ν_{max} ($CHCl_3$) 3398, 2870, 1452, 1355, 1063 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$, TMSCl): δ 2.97 (s, 1H, OH), 3.29 (s, 3H, OCH_3), 3.59 (dd, *J* = 11.7, 8.4, 1H, CH_{2B}OH), 3.69 (dd, *J* = 11.7, 3.9, 1H, CH_{2A}OH), 4.3 (dd, *J* = 8.4, 3.9, 1H, C*H*OCH_3), 7.23-7.38 (m, 5H, H-*aromatic*), ^{13}C NMR (300 MHz; $CDCl_3$): δ 56.7 (CH_3), 67.2 (CH_2), 84.8 (CH), 126.7 (*ortho*), 128.0 (*para*), 128.4 (*meta*), 138.3 (*ipso*); *m/z* (EI) 153 (M^+, 5%), 135 (10), 121 (100).

2-Ethoxy-2-phenylethanol, IR ν_{max} ($CHCl_3$) 3589,3011, 2978, 1101, 1032 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.21 (t, *J* = 6.9, 3H, CH_3), 2.93 (br s, 1H, OH), 3.34-3.57 (m, 2H, OCH_2CH_3), 3.58 (dd, *J* = 11.7, 3.9, 1H, CH_{2B}OH), 3.66 (dd, *J* = 11.7, 8.4, 1H, CH_{2A}OH), 4.40 (dd, *J* = 8.4, 3.9, $CHOCH_2CH_3$), 7.24-7.36 (m, 5H, H-*aromatic*). ^{13}C NMR (300 MHz; $CDCl_3$): δ 15.1 (CH_3), 64.3 (CH_2CH_3), 67.1 (CH_2OH), 82.8 ($CHOCH_2CH_3$), 126.6 (*ortho*), 127.8 (*para*), 128.3 (*meta*), 138.9 (*ipso*); *m/z* (EI) 149 (M^+, 10%), 135 (100), 107 (60), 79 (60).

2-Phenyl-2-propoxyethanol, IR ν_{max} ($CHCl_3$) 3588, 2965, 2878, 1101, 1031 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.92 (t, *J* = 7.5, 3H, CH_3), 1.62 (sx, *J* = 7.5, 2H, CH_2CH_3), 2.87 (s, 1H, OH), 3.28-3.42 (m, 2H, $OCH_2CH_2CH_3$), 3.59 (dd, *J* = 11.7, 4.2, 1H, CH_{2B}OH), 3.68 (dd, *J* = 11.7, 8.3, 1H, $CH_{2A}OH$), 4.40 (dd, *J* = 8.3, 4.2, 1H, C*H*OCH_2), 7.26-7.38 (m, 5H, H-*aromatic*), ^{13}C NMR (300 MHz; $CDCl_3$): δ 10.4 (CH_3), 22.9 ($CH_2CH_2CH_3$), 67.2 ($OCH_2CH_2CH_3$), 70.7 (OCH_2OH), 82.8 (*C*HOH), 126.6 (*ortho*), 127.8 (*para*), 128.3 (*meta*) 139.0 (*ipso*); *m/z* (EI) 181 (M^+, 5%), 165 (20), 150 (100), 122 (60), 108 (98), 91 (25), 79 (50).

2-*iso*-Propoxy-2-phenylethanol, IR ν_{max} ($CHCl_3$) 3586, 3009, 2975, 1117, 1030 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.16 (d, *J* = 6.0, 3H, CH_3), 1.23 (d, *J* = 6.0, 3H, CH_3), 3.13 (s, 1H, OH), 3.57-3.71 (m, 3H, O*CH*$(CH_3)_2$, CH_2OH), 4.56 (dd, *J* = 8.1, 3.9, C*H*$OCH(CH_3)_2$, 7.28-7.37 (m, 5H, *aromatics*), ^{13}C NMR (300 MHz; $CDCl_3$): δ 21.0 (CH_3), 23.1 (CH_3), 67.1 (CH_2OH), 69.1 ($OCH(CH_3)_2$), 79.9 ($CHOCH(CH_3)_2$), 126.5 (*ortho*), 127.5 (*para*), 128.1 (*meta*), 139.6 (*ipso*); *m/z* (EI) 181 (M^+, 2%), 150 (40), 122 (20), 108 (100), 79 (50).

2-Butoxy-2-phenylethanol, IR ν_{max} ($CHCl_3$) 3588, 2958, 2935, 1100, 1031 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.95 (t, *J* = 7.5, 3H, CH_3), 1.36-1.49 (m, 2H, CH_2CH_3), 1.59-1.68 (m, 2H, C$H_2CH_2CH_3$), 2.51 (s, 1H, OH), 3.37 (dt, *J* = 9.3, 6.3, OCH_{2B}), 3.49 (dt, *J* = 9.3, 6.3, OCH_{2A}), 3.62-3.75 (m, 2H, CH_2OH), 4.45 (dd, *J* = 8.4, 4.3, C*H*OCH_2), 7.31-7.43 (m, 5H *aromatics*), ^{13}C NMR (300 MHz; $CDCl_3$): δ 13.9 (CH_3), 19.3 (CH_2CH_3), 31.9 (C$H_2CH_2CH_3$), 67.4 (CH_2OH), 68.9

(OCH_2), 82.8 (*C*$HOCH_2$), 126.8 (*ortho*), 128.0 (*para*), 128.4 (*meta*), 139.0 (*ipso*); *m/z* (EI) 195 (M^+, 40%), 177 (50), 163 (70), 121 (100), 91 (30).

2-*sec*-Butoxy-2-phenylethanol (inseparable mixture of diastereomers), IR ν_{max} ($CHCl_3$) 3586,2966, 2879, 1092, 1057 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.82 (t, 3H, *J* = 7.5, **CH_2CH_3**), 0.90 (t, 3H, *J* = 7.5, CH_3), 1.03 (d, 3H, *J* = 6.3, $CHCH_3$), 1.15 (d, 3H, *J* = 6.3, **$CHCH_3$**), 1.24-1.64 (m, 4H, **CH_2CH_3**, CH_2CH_3), 2.36 (s, 1H, **OH**, OH), 3.24-3.45 (m, 2H, **$OCH(CH_3)CH_2CH_3$**, $OCH(CH_3)CH_2CH_3$), 3.51-3.67 (m, 4H, **CH_2OH**, CH_2OH), 4.42-4.5 (m, 2H, **$PhCHOCH(CH_3)CH_2CH_3$**, $PhCHOCH(CH_3)CH_2CH_3$), 7.19-7.26 (m, 10H, ***aromatics***), ^{13}C NMR (300 MHz; $CDCl_3$): δ 9.3 (CH_3), 10.1 (**CH_3**), 18.6 ($CHCH_3$), 20.3 (**CH_2CH_3**), 28.1 ($CHCH_2CH_3$), 30.2 (**$CHCH_2CH_3$**), 67.4 ($CH_2OCH(CH_3)CH_2CH_3$), 67.5 (**CH_2OH**), 73.9 (**$OCH(CH_3)CH_2CH_3$**), 75.1 ($OCH(CH_3)CH_2CH_3$), 79.5 (**$CHOCH(CH_3)CH_2CH_3$**), 80.6 (*C*HOH), 126.8 (***ortho***), 127.1 (*ortho*), 127.8 (***para***), 127.9 (*para*), 128.3 (***meta***, *meta*), 139.4 (***ipso***), 139.9 (*ipso*); *m/z* (EI) 195 (M^+, 10%), 177 (20), 163 (40), 121 (100), 107 (70), 79 (45).

2-*tert*-Butoxy-2-phenylethanol, mp: 67-68 °C. IR ν_{max} ($CHCl_3$) 3586, 2977, 1369, 1060 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$, TMSCl): δ 1.17 (s, 9H, 3 x CH_3), 2.01 (s, 1H, OH), 3.48 (dd, *J* = 11.4, 8.4, 1H, $CH_{2B}OH$), 3.52 (dd, *J* = 11.4, 4.2, 1H, $CH_{2A}OH$) 4.62 (dd, *J* = 8.4, 4.2, 1H, ($CHOC(CH_3)_3$), 7.25-7.36 (m, 5H, H *aromatic*), ^{13}C NMR (300 MHz; $CDCl_3$): δ 28.8 (3 x CH_3), 67.9 (CH_2), 74.9 ($OC(CH_3)_3$), 75.1 (CH), 126.3 (*ortho*), 127.3 (*para*), 128.2 (*meta*), 142.2 (*ipso*); m/z (EI) 194 (M^+, 3%), 163 (15), 121 (10), 107 (100), 79 (20).

1-Methoxybutan-2-ol (bold) and 2-Methoxybutan-1-ol (inseparable mixture of regioisomers), IR ν_{max} ($CHCl_3$, of mixture) 3585, 2970, 2935, 1462, 1087 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.88 (t, *J* = 7.5, 3H, CH_3), 0.93 (t, *J* = 7.5, 3H, **CH_3**), 1.40-1.48 (m, 2H, CH_2CH_3), 1.49-1.64 (m, 2H, **CH_2CH_3**), 2.15 (s, 1H, **OH**, OH), 3.14-3.71 (m, 6H, **CH_2OCH_3**, **CHOH**, CH_2OH, $CHOCH_3$), 3.35 (s, 3H, OCH_3), 3.38 (s, 3H, **OCH_3**); ^{13}C NMR (300 MHz; $CDCl_3$): δ 9.5 (**CH_3**), 9.9 (CH_3), 22.9 (CH_2CH_3), 26.0 (**CH_2CH_3**), 57.0 (**OCH_3**), 59.0 (OCH_3), 63.5 (CH_2OH), 71.6 (**CHOH**), 76.6 (**CH_2OCH_3**), 82.8 ($CHOCH_3$); m/z (CI) 105 ($[M+1]^+$, 100%), 87 (70), 73 (45).

1-Ethoxybutan-2-ol (bold) and **2-Ethoxybutan-1-ol (as an inseparable mixture of regioisomers),** IR ν_{max} ($CHCl_3$) 3583, 3009, 2976, 2880, 1107 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.83 (t, *J* = 7.3, 3H, $CHCH_2CH_3$), 0.88 (t, *J* = 7.2, 3H, **$CHCH_2CH_3$**), 1.32 (t, *J* = 7.1, 3H, **OCH_2CH_3**), 1.32 (t, *J* = 7.1, 3H, OCH_2CH_3), 1.35-1.43 (m, 2H, $CHCH_2CH_3$), 1.45-1.57 (m, 2H, **$CHCH_2CH_3$**), 2.60 (s, 2H, **OH**, OH), 3.16-3.24 (m, 2H, $OCH_{2B}CH_3$, $CHOCH_2CH_3$), 3.35-3.66 (m, 8H, **OCH_2CH_3**, **$CH_2OCH_2CH_3$**, **CHOH**, CH_2OH, $OCH_{2A}CH_3$), ^{13}C NMR (300 MHz; $CDCl_3$): δ 9.5 (**$CHCH_2CH_3$**), 9.7 (CH_2CH_3), 14.9 (OCH_2CH_3), 15.4 (**OCH_2CH_3**), 23.4 (CH_2CH_3), 26.0 (**$CHCH_2CH_3$**), 63.7 (**OCH_2CH_3**), 64.7 (CH_2OH), 66.6 (**$CH_2OCH_2CH_3$**), 71.5 (**CHOH**), 74.5 (OCH_2CH_3), 81.1 ($CH_2OCH_2CH_3$); m/z (CI) 119 ($[M+1]^+$, 100%), 101 (80), 73 (40).

1-*iso*-Propoxybutan-2-ol (bold) and 2-*iso*-Propoxybutan-1-ol (as an inseparable mixture of regioisomers), IR ν_{max} ($CHCl_3$) 3580, 3009, 2978, 1128, 1071 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.81 (t, *J* = 7.4, 3H, CH_2CH_3), 0.86 (t, *J* = 7.5, 3H, **CH_2CH_3**), 1.06 (t, *J* = 6.0, 6H, $OCH(CH_3)_2$), 1.06 (t, *J* = 6.0, 6H, **$OCH(CH_3)_2$**), 1.46-1.32 (m, 4H, **CH_2CH_3** and CH_2CH_3), 2.74 (s, 2H, **OH,** OH), 3.08-3.65 (m, 8H, **$CH_2OCH(CH_3)_2$**, **$OCH(CH_3)_2$**, **CHOH**, $OCH(CH_3)_2$, CH_2OH, $OCH(CH_2)_2$), ^{13}C NMR (300 MHz; $CDCl_3$): δ 9.6 (**CH_2CH_3**), 9.7 (CH_2CH_3), 21.8 (**$CH(CH_3)$**), 21.9 ($CH(CH_3)$), 22.5 (**$CH(CH_3)$**), 22.7 ($CH(CH_3)$), 24.2 (CH_2CH_3), 25.9 (**CH_2CH_3**), 64.0 (CH_2OH), 70.0 (**CHOH**), 71.6 (**$OCH(CH_3)$**), 71.8 ($CH(CH_3)_2$), 72.0 (**$CH_2OCH(CH_3)_2$**), 72.5 ($OCH(CH_2)_2$); m/z (CI) 132 ($[M]^+$, 80%), 115 (20), 73 (100).

2-Methoxycyclohexanol, IR ν_{max} ($CHCl_3$) 3566, 2920, 2829, 1120, 1080 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$) δ 1.12 (m, 1H, $H6_B$), 1.18-1.30 (m, 3H, $H3_B$, $H4_B$, $H5_B$), 1.65-1.69 (m, 1H, 5_A), 1.71-1.75 (m, 1H, $H4_A$), 1.94-2.01 (m, 1H, $H6_A$), 2.06-2.13 (m, 1H, $H3_A$), 2.92 (ddd, *J* = 10.5, 8.7, 4.5, 1H. C*H*OCH_3), 2.99 (s, 1H, OH), 3.38 (s, 3H, OCH_3), 3.35-3.45 (m, 1H, C*H*OH), ^{13}C NMR (300 MHz; $CDCl_3$): δ 23.8 (C5), 23.9 (C4), 28.2 (C6), 32.0 (C3), 56.1 (O*C*H3), 73.4 (*C*HOH), 84.8 (*C*HOCH3); m/z (EI) 131 (M^+, 20%), 113 (15), 98 (25), 84 (35), 71 (100).

2-Ethoxycyclohexanol, IR ν_{max} ($CHCl_3$) 3579, 2970, 1451, 1090 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.17 (t, *J* = 7.2, 3H, CH_3), 1.15-1.22 (m, 4H, $H3_B$, $H4_B$, $H5_B$, $H6_B$), 1.63-1.70 (m, 2H, $H4_A$, $H5_A$), 1.93-2.06 (m, 2H, $H3_A$, $H6_A$), 2.81 (s, 1H, OH), 2.97 (ddd, *J* = 10.5, 8.7, 4.5, 1H, C*H*OCH_2CH_3), 3.32-3.43 (m, 2H, HOC*H*, O*C*H_{2B}), 4.12 (dq, *J* = 7.2, 0.9, 1H, OCH_{2A}), ^{13}C NMR (300 MHz; $CDCl_3$): δ 15.6 (CH_3), 23.9 (C4 or C5), 24.2 (C4 or C5), 29.1 (C3 or C6), 31.9 (C3 or C6), 64.0 (O*C*H_2CH_3), 71.6 (C1), 83.4 (C2); *m/z* (EI) 145 (M^+, 20%), 127 (100), 85 (25), 81 (35), 57 (20).

2-Propoxycyclohexanol, IR ν_{max} ($CHCl_3$) 3578, 2876, 1452, 1099, 1076 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.84 (t, *J* = 7.1, 3H, CH_3), 1.00-1.24 (m, 1H, H_{3B}, H_{4B}, H_{5B}, H_{6B}), 1.50 (br sx, *J* = 7.0, 2H, C*H*$_2$$CH_3$), 1.56-1.68 (m, 2H, H_{4A}, H_{5A}), 1.88-2.41 (m, 2H, H_{3A}, H_{6A}), 2.80 (s, OH), 2.92 (ddd, *J* = 10.5, 8.8, 4.3, 1H, C*H*O$CH_2CH_2CH_3$), 3.35 (dt, *J* = 9.3, 6.7, 1H, OC*H*$_{2B}$), 3.28-3.37 (m, 1H, C*H*OH), 3.39 (dt, *J* = 9.3, 6.7, 1H, OC*H*$_{2A}$); ^{13}C NMR (300 MHz; $CDCl_3$): δ 10.4 (CH_3), 23.2 (CH_2CH_3), 23.8 (C5), 24.1 (C4), 29.0 (C6), 31.9 (C3), 70.3 (O*C*H_2), 73.6 (*C*HOH), 83.4 (*C*HOCH_2); *m/z* (EI) 181 (M^+, 2%), 159 (50), 141 (100), 99 (50), 81 (50).

2-*iso*-Propoxycyclohexanol, IR ν_{max} ($CHCl_3$) 3455, 2853, 1454, 1134, 1039 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.08 (d, *J* = 6.1, 3H, CH_3), 1.12 (d, *J* = 6.1, 3H, CH_3), 1.09-1.14 (m, 2H, H_{5B}, H_{6B}), 1.16-1.66 (m, 4H, H_{3B}, H_{4A}, H_{4B}, H_{5A}), 1.90-1.92 (m, 1H, H_{6A}), 1.93-1.97 (m, 1H, H_{3A}), 2.66 (s, 1H, OH), 2.96-3.04 (m, 1H, C*H*O$CH(CH_3)_2$), 3.26-3.34 (m, 1H, C*H*OH), 3.67 (septet, *J* = 6.1, 1H, C*H*$(CH_3)_2$). ^{13}C NMR (300 MHz; $CDCl_3$): δ 22.1 (CH_3), 23.7 (CH_3), 23.9 (C4 or C5), 24.3 (C4 or C5), 30.2 (C3 or C6), 31.9 (C3 or C6), 69.4 (*C*H$(CH_3)_2$), 73.6 (*C*HOH), 81.2 (*C*HOCH); m/z (EI) 159 (M^+, 95%), 143 (100).

2-Butoxycyclohexanol, IR ν_{max} ($CHCl_3$) 3579, 2976, 2932, 1080, 1093 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.86 (t, *J* = 6.9, 3H, CH_3), 1.01-1.13 (m, 1H, H_{6B}), 1.15-1.23 (m, 3H, H_{3B}, H_{4B}, H_{5B}), 1.27-1.37 (m, 2H, C*H*$_2$$CH_3$), 1.45-1.54 (m, 2H, OCH_2C*H*$_2$), 1.60-1.63 (m, 1H, H_{5A}), 1.65-1.67 (m, 1H, H_{4A}), 1.90-1.95 (m, 1H, H_{6A}), 1.97-2.03 (m, 1H, H_{3A}), 2.62 (s, 1H, OH), 2.93 (ddd, *J* = 10.5, 8.7, 4.5, 1H, C*H*OCH_2), 3.22 (dt, *J* = 9.2, 6.6, 1H, OC*H*$_{2B}$), 3.38-3.30 (m, 1H, C*H*OH), 3.51 (dt, *J* = 9.2, 6.6, 1H, OC*H*$_{2A}$). ^{13}C NMR (300 MHz; $CDCl_3$): δ 13.8 (CH_3), 19.3 (CH_2CH_3), 23.9 (C5), 24.2 (C4), 29.1 (C6), 31.9 (C3), 32.2 (*C*H$_2$$CH_2CH_3$), 68.4 ($OCH_2$), 73.8 (*C*HOH), 83.6 (*C*HOCH_2); m/z (EI) 173 (M^+ 40%), 155 (100), 133 (10), 99 (20), 81 (30), 57 (25).

2-sec-Butoxycyclohexanol (inseparable mixture of diastereomers), IR ν_{max} ($CHCl_3$) 3582, 2970, 2931, 1077, 1070 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.86 (t, *J* = 7.4, 3H, **CH_2C*H*$_3$**), 0.87 (t, *J* = 7.4, 3H, CH_2C*H*$_3$), 1.08 (t, *J* = 2.7, OCHC*H*$_3$), 1.10 (t, *J* = 2.7, 3H, **OCHC*H*$_3$**), 1.12-1.24 (m, 8H, **$CH_{2B}$$CH_3$**, **$CH_{2B}$-3**, **$CH_{2B}$-4**, **$CH_{2B}$-6**, $CH_{2B}CH_3$, CH_{2B}-3, CH_{2B}-4, CH_{2B}-6), 1.34-1.65 (m, 8H, **$CH_{2A}CH_3$**, **CH_{2A}-4**, **CH_2-5**, $CH_{2A}CH_3$, CH_{2A}-4, CH_2-5), 1.91-2.00 (m, 4H, **CH_{2A}-3**, **CH_{2A}-6**, CH_{2A}-3, CH_{2A}-6), 2.77 (s, 1H, **OH**, OH), 2.97-3.07 (m, 2H, ***C*HOCHCH$_3$**, *C*HOCHCH$_3$), 3.29-3.50 (m, 4H, **C*H*OH**, **C*H*CH3**, C*H*OH, C*H*CH3); ^{13}C NMR (300 MHz; $CDCl_3$): δ 9.8 (**CH_2*C*H$_3$**), 10.2 (CH_2*C*H$_3$), 19.8 (CH*C*H$_3$), 21.0 (**CH*C*H$_3$**), 23.9 (*C*H$_2$CH$_3$), 24.7 (***C*H$_2$CH$_3$**), 29.3 (**C5**), 29.9 (C5), 30.3 (**C4**, C4), 30.7 (**C6**, C6), 31.9 (**C3**, C3), 73.6 (***C*HCH$_3$**), 74.0 (*C*HCH$_3$),

74.3 (C1), 75.4 (**C1**), 80.9 (C2), 82.2 (**C2**). m/z (EI) 173 (M^+, 90%), 155 (40), 177 (45), 99 (70), 81 (90).

2-tert-Butoxycyclohexanol, mp 27-28 °C. IR ν_{max} ($CHCl_3$) 3488, 2978, 2939, 1193, 1066 cm^{-1}; ^1H NMR (300 MHz; $CDCl_3$): δ 1.22 (s, 9H, CH_3), 1.19-1.25 (m, 4H, H_{3B}, H_{4B}, H_{5B}, H_{6B}), 1.60-1.66 (m, 2H, H_{4A}, H_{5A}), 1.86-1.92 (m, 1H, H_{6A}), 1.98-2.03 (m, 1H, H_{3A}), 2.51 (s, 1H, OH), 3.14-3.22 (m, 1H, C*H*OC$(CH_3)_3$), 3.24-3.33 (m, 1H, C*H*OH); ^{13}C NMR (300 MHz; $CDCl_3$): δ 24.2 (C5), 24.7 (C4), 29.1 (3 x CH_3), 32.1 (C6), 33.4 (C3), 73.9 (*C*HOH), 74.0 (*C*$(CH_3)_3$), 76.5 (*C*HOC$(CH_3)_3$); m/z (CI) 173 (M^+, 10%), 155 (10), 117 (20), 99 (100), 81 (30).

2-Ethoxycyclododecanol, mp 61.5-62.5 °C. IR ν_{max} ($CHCl_3$) 3562, 2933, 2866, 1446, 1098 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.19 (t, *J* = 6.9, 3H, CH_3), 1.32-1.42 (m, 16H, 8 x CH_2), 1.61-1.75 (m, 4H, C*H*$_2$CHOH, C*H*$_2$CHOCH_2CH$_3$), 2.42 (s, 1H, OH), 3.40 (dq, *J* = 9.3, 7.4, 1H, OC*H*$_{2B}$CH$_3$), 3.63-3.73 (m, 2H, HCOH, OC*H*$_{2A}$CH$_3$), ^{13}C NMR (300 MHz; $CDCl_3$): δ 15.6 (CH_2*C*H$_3$), 19.6, 22.2, 22.76 (2C), 22.80, 23.2, 24.6, 25.0, 25.9, 29.3 (10 x CH_2, C3-C12), 64.8 (O*C*H$_2$CH$_3$), 69.5 (*C*HOH), 80.5 (*C*HOCH$_2$CH$_3$). m/z (EI) 229 (M^+, 2%), 227 (20), 199 (20), 183 (20), 55 (100).

2-Butoxycyclododecanol, mp 43.5-44.5 °C. IR ν_{max} ($CHCl_3$) 3557, 3015, 1233, 789, 711 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 0.90 (t, *J* = 7.4, 3H, CH$_2$C*H*$_3$), 1.32-1.77 (m, 24H, 10CH$_2$, OCH$_2$C*H*$_2$C*H*$_2$CH$_3$), 2.65 (s, 1H, OH), 3.20-3.24 (m, 1H, C*H*O$(CH_2)_3$CH$_3$), 3.31 (dt, *J* = 9.3, 6.5 (OC*H*$_{2B}$$(CH_2)_2CH_3$), 3.64 (dt, *J* = 9.3, 6.5 (OC*H*$_{2A}$$(CH_2)_2CH_3$), 3.70 (dt, *J* = 5.3, 2.4, C*H*OH), ^3C NMR (300 MHz; $CDCl_3$): δ 13.9 (CH_3), 19.4, 19.5, 22.2 , 22.8 (3C), 23.1, 24.7, 25.1, 25.7, 29.3, 32.2 (12C, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, OCH$_2$C*H*$_2$C*H*$_2$CH$_3$), 69.2 (O*C*H$_2$), 69.6 (*C*HOH), 80.6 (*C*HOCH$_2$$(CH_2)_2CH_3$); m/z (CI) 257 ($[M+1]^+$, 45%), 239 (100), 183 (50), 165 (25).

1-Allyoxy-3-ethoxy-propan-2-ol, IR **ν_{max}** ($CHCl_3$) 3578, 2975, 2881, 1647, 1097 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.13 (t, *J* = 7.1, 3H, CH_3), 2.78 (s, 1H, OH), 3.34-3.50 (m, 6H, OC*H*$_2$CHOH, OC*H*$_2$CH$_3$, C*H*$_2$OCH$_2$CH$_3$), 3.85-3.92 (m, 1H, C*H*OH), 3.94 (dt, *J* = 5.6, 1.5, 2H, CH$_2$=CHC*H*$_2$), 5.10 (app dq, *J* = 10.5, 1.5, 1H, HC=C*H*$_{2B}$), 5.20 (app dq, *J* = 17.3, 1.5, HC=C*H*$_{2A}$), 5.83 (ddt, *J* = 17.3, 10.5, 5.6, 1H, *H*C=CH$_2$); ^{13}C NMR (300 MHz; $CDCl_3$): δ 15.0 (CH_3), 66.7 (O*C*H$_2$CH$_3$), 69.3 (*C*HOH), 71.3 (*C*H$_2$OCH$_2$CH$_3$ or OCH$_2$CHOH), 71.6 (OCH$_2$CHOH or *C*H$_2$OCH$_2$CH$_3$), 72.1 (HC=CH$_2$*C*H$_2$), 116.9 (HC=*C*H$_2$), 134.4 (H*C*=CH$_2$); ***m/z*** (EI) 161 (M^+ 40%), 103 (35), 87 (45), 71 (35), 59 (100).

1-tert-Butoxy-3-ethoxy-propan-2-ol, IR **ν_{max}** ($CHCl_3$) 3576, 2971, 1366, 1191, 1082 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.16 (s, 9H, 3 x CH_3), 1.18 (t, *J* = 6.9, 3H, CH$_2$C*H*$_3$), 2.40 (s, 1H, OH), 3.31-3.90 (m, 7H, C*H*OH, OC*H*$_2$CH$_3$, C$(CH_3)_3$OC*H*$_2$, C*H*$_2$OCH$_2$CH$_3$);^{13}C NMR (300 MHz; $CDCl_3$): δ 15.1 (OCH$_2$*C*H$_3$), 27.5 (3 x CH_3), 62.9 (O*C*H$_2$CH$_3$), 66.8 (C$(CH_3)_3$O*C*H$_2$), 69.9 (*C*HOH), 71.7 (*C*H$_2$OCH$_2$CH$_3$), 78.2 (*C*$(CH_3)_3$); ***m/z*** (EI) 177 (M^+, 40%), 121 (100), 103 (15), 57 (25).

1-Ethoxy-3-phenoxy-propan-2-ol, IR **ν_{max}** ($CHCl_3$) 3586, 2979, 1495, 1120 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.21 (t, *J* = 6.9, 3H, CH_3), 3.07 (br s, OH), 3.50-3.65 (m, 4H, OC*H*$_2$CH$_3$, C*H*$_2$OCH$_2$CH$_3$), 3.97-4.06 (m, 2H, CHOC*H*$_2$), 4.13-4.20 (m, 1H, C*H*OH), 6.90-7.00 (m, 3H, H*o*,*p*-aromatic), 7.24-7.30 (m, 2H, H*m*-aromatic); ^{13}C NMR (300 MHz; $CDCl_3$): δ 15.0 (OCH$_2$*C*H$_3$), 66.9 (O*C*H$_2$CH$_3$), 68.9 (*C*H$_2$OCH$_2$CH$_3$), 69.0 (CH), 71.28 (Ph-O*C*H$_2$), 114.5 (*ortho*),

120.9 (*para*), 129.4 (*meta*), 158.5 (*ipso*); *m/z* (EI) 196 (M^+, 100%), 195 (30), 133 (35), 94 (70), 77 (45), 59 (100), 51 (30).

1-Ethoxy-3-(4-oxiranylmethoxy-butoxy)-propan-2-ol, IR ν_{max} ($CHCl_3$) 3577, 2916, 1252, 1081, 909 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.16 (t, *J* = 6.9, 3H, CH_3), 1.59-1.61 (m, 4H, $OCH_2CH_2CH_2CH_2O$), 2.40 (br s, OH), 2.56 (dd, *J* = 5.0, 2.6, 1H, oxirane $CH_{2B}OCHCH_2$), 2.74 (t, *J* = 5.0, 1H, oxirane $CH_{2A}OCHCH_2$), 3.07-3.12 (m, 1H, oxirane CH_2OCHCH_2), 3.31-3.73 (m, 12H, OCH_2CH_3, $CH_2OCH_2CH_3$, OCH_2CHOH, $CH_2CH_2OCH_2$ x 2, $CHCH_2OCH_2$), 3.85-3.93 (m, 1H, CHOH), ^{13}C NMR (300 MHz; $CDCl_3$): δ 14.7 (CH_3), 25.9 (CH_2CH_2), 26.0 (CH_2CH_2), 43.8 ($CHOCH_2$ oxirane), 50.5 ($CHOCH_2$ oxirane), 66.4 (OCH_2CH_3), 69.0 (CHOH), 70.77 (OCH_2), 70.82 (OCH_2), 71.0 (OCH_2), 71.5 (OCH_2), 71.7 (OCH_2); *m/z* (EI) 249 ($[M+1]^+$, 10%), 175 (10), 129 (100), 103 (35).

2-Ethoxy-3-[4-(2-ethoxy-3-hydroxy-propoxy)-butoxy]-propan-1-ol, IR ν_{max} ($CHCl_3$) 3577, 2901, 1243, 1143, 1129 cm^{-1}. ^1H NMR (300 MHz; $CDCl_3$): δ 1.13 (t, *J* = 6.9, 6H, 2 x CH_3), 1.54-1.60 (m, 4H, 2 x CH_2), 2.78 (s, 2H, 2 x OH), 3.33-3.49 (m, 16H, 2 x OCH_2CH_3, 2 x $CH_2OCH_2CH_3$, 2 x CH_2OCH_2CHOH, 2 x CH_2OCH_2CHOH), 3.90 (m, 2H, 2 x CHOH), ^{13}C NMR (300 MHz; $CDCl_3$): δ 15.0 (2 x CH_3), 26.1 ($OCH_2CH_2CH_2CH_2O$), 66.7 (2 x OCH_2CH_3), 69.3 (2 x CHOH), 71.1 (2 x OCH_2), 71.6 (2 x OCH_2), 71.9 (2 x OCH_2); *m/z* (EI) 294 (M^+, 40%), 175 (100), 147 (15), 115 (30), 59 (40).